

Aspirin  
50-78-2 | DTXSID5020108

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

## Model Results

**Predicted value:** 125 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 9.29e-01

**Confidence level:** 4.97e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Aspirin

**Measured:** 135

**Predicted:** 125

[Image not found](#)

Monomethyl phthalate

**Measured:** 83.0

**Predicted:** 116

[Image not found](#)

Benzoic acid, 4-(acetyloxy)-

**Measured:** 193

**Predicted:** 140

[Image not found](#)

Monobutyl phthalate

**Measured:** 73.5

**Predicted:** 96.8